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Autor: Bartolini, A. / Ercolessi, F. / Tosatti, E.
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MAGIC VICINAL SURFACES INDUCED BY RECONSTRUCTION

A. Bartolini, F. Ercolessi, and E. Tosatti, Int. School for Advanced Studies
I-34014 TRIESTE, Italy

Abstract: We have studied the structure and surface energetics of vicinals of Au(100) and Au(111), using a well-tested many-body force model for gold. Surface reconstruction takes place on terraces between steps, causing the appearance of particularly favoured "magic" orientations whenever the terrace width roughly contains an integer number of reconstruction cells. Implications on the faceting behaviour of these surfaces are discussed.

Usually, the surface energy σ of a vicinal surface is determined simply by its density of steps, which is proportional to the tilting angle θ. Therefore, for small θ (where step-step interactions can be neglected), σ behaves like $\sigma_0 + k|\theta|$, where k is proportional to the step energy. However, when the low-index surface reconstructs the large terraces between two steps may also become reconstructed. This can yield new surface energy terms which are minimal whenever terraces contain an integer number N of unit cells, leading to rather stable "magic" orientations, with an energy lower than neighbouring orientations.

We have investigated the T=0 structure and energetics of vicinals of Au(100) and Au(111)—both of which exhibit long-period reconstructions. We have used the well-tested "glue" many-body force model [1] and a simulated-annealing energy minimization procedure based on molecular dynamics. Reconstruction is included by allowing the terraces to become laterally denser, as was previously found to be optimal on flat Au(100) and Au(111) in the same model [1]. We have found that in both cases there is indeed reconstruction-related structure in the surface energy $\sigma(\theta)$, and magic vicinals are present.

Results for the (K11), K-odd family of Au(100) vicinals are reported in Fig. 1. (11,1,1), (511) and (311) are particularly stable, and all the other vicinals of the family improve their surface energy by faceting into a suitable combination of (100), (11,1,1) and (511). This result, obtained without any adjustable parameters, agrees strikingly with recent LEED data, which indicate precisely (11,1,1), (511) and (311) as the preferred vicinals of Au(100) [2]. The stability of (11,1,1) is to be related with the onset of an optimally dense triangular reconstruction on each terrace, similar to the $\sim (1 \times 5)$ reconstruction of Au(100). Steps remain sharp and well-defined. In the case of (511) and (311), relaxation transforms the ideal step/terrace structure into a corrugated, dense nearly-triangular overlayer. Here, the increase of surface packing is a consequence of the decrease of the microscopic surface area arising from step flattening.

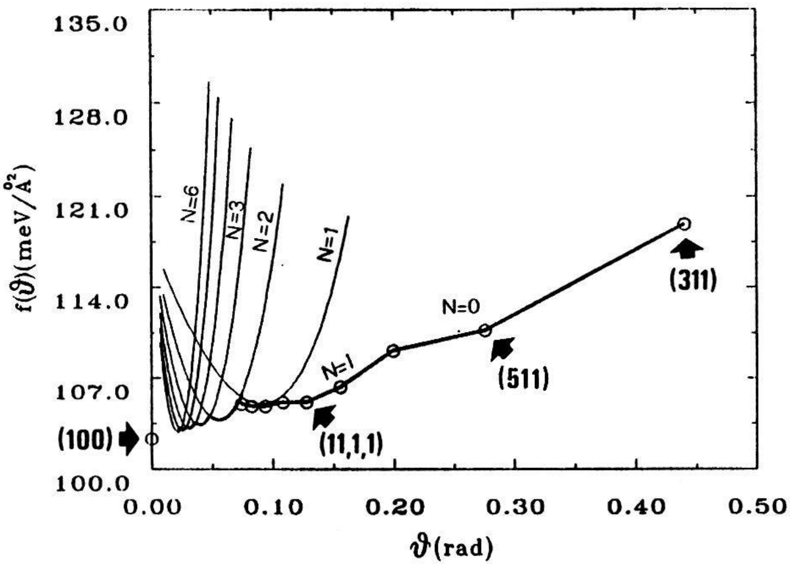

Figure 1: Surface energy of Au(K11) (100)-vicinals referred to the (100)-projected area, $f(\theta) = \sigma(\theta)/\cos(\theta)$, as a function of θ. The points represent results obtained by energy minimization. The thin lines are obtained by a simple analytical model reproducing other points (not shown) obtained for small θ. Each curve corresponds to a different number N of reconstruction cells within each terrace. The lower, thick envelope curve, representing stable states, has cusps in correspondence with transitions between different values of N. Note the particular stability of (511) and (11, 1, 1). The point at $\theta = 0$ is the surface energy of (1×5) reconstructed Au(100), from previous work [1].

A similar surface energy analysis performed for the $(\mathrm{M}+1, \mathrm{M}-1, \mathrm{M})$ family of Au(111) vicinals shows that groups of magic orientations appear when $\mathrm{M} \sim 11, 22, \ldots$, i.e. when the terrace length is multiple of the reconstruction cell length predicted by the model [1]. This result allows an immediate interpretation of STM observations of groups of steps on flat Au(111), arranged in a regular array whose spacing seems to correspond exactly with the basic reconstruction periodicity [3].

In conclusion, we have found that long-period surface reconstructions lead to the appearance of particularly stabilized, "magic" vicinal surfaces. We expect this phenomenon to be quite general, and to occur also on other reconstructing surfaces.

References

[1] F. Ercolessi, A. Bartolini, M. Garofalo, M. Parrinello and E. Tosatti, Physica Scripta T19, 399 (1987), and references therein.

[2] M. Sotto and J. C. Boulliard, preprint (1989).

[3] W. J. Kaiser and R. C. Jaklevic, Surface Sci. 182, L227 (1987).